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TECHNICAL REPORT RD-82-2

COMPBL-II - COMPRESSIBLE, VARIABLE PRESSURE
BOUNDARY LAYER PROGRAM FOR ARBITRARY GASEOUS
MIXTURES

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SYMBOLS

a	Sonic Velocity
C*	Sonic Speed at M = 1
C _{pi}	Specie Specific Heat
C _{p mix}	Mixture Specific Heat
k _i	Thermal Conductivity of Specie
k _{mix}	Thermal Conductivity of the Mixture
M	Mach Number
MW mix	Molecular Weight of Gas Mixture
P	Prandtl Number
$\frac{R}{MW}$	Universal Gas Constant = 8314.3 J/Kmole °K
Re	Reynolds Number
T	Temperature
U	Streamwise Velocity Component
W	Viscosity Power Law Exponent
Y _i	Elemental Mole Fraction
p	Pressure
ρ	Density
μ	Absolute Viscosity
M*	Dimensionless Speed Ratio M* = u/c*

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I. INTRODUCTION

The compressible flow boundary layer program, COMPBL¹, was written to calculate the two dimensional boundary layer flow for an arbitrary pressure gradient in air. An integral technique based on the Walz² method was utilized in this program. Capabilities include axisymmetric/plane geometry, laminar/turbulent flow, incompressible/compressible flow, with or without heat transfer. This program was written for the CDC CYBER class of computers and is in use locally in the BATCH mode.

There are two deficiencies of this code as it presently is used:

A. It is limited to boundary layer flows in air.

B. It has limited usefulness as an aero design tool since it is utilized in a BATCH mode.

These two deficiencies were corrected in this analysis and resulted in COMPBL-II which has the following additional capabilities:

A. Allows an arbitrary chemical composition of the boundary layer flow.

B. Runs either interactively on the INTERDATA 8/32 or BATCH on the CYBER Series.

II. ANALYSIS

The chemical species chosen for use in this analysis were taken from the DATABANK subroutine of the JANNAF Standardized Plume Flowfield (SPF) Code. These include those of most interest for rocket calculation. It was necessary to utilize transport property data for the chemical species chosen in order to calculate the boundary layer for internal flows. These data were tabulated over a wide range of temperatures (200-3700 °K) covering both internal and external flows. These data include:

A. Elemental viscosity, μ_i

B. Thermal conductivity, k_i

C. Constant pressure specific heat, C_{p_i}

Data a and b were taken directly from NASA TR-R-132³. Data c was taken from the DATABANK subroutine of the SPF code and include coefficients of a curve fit of C_{p_i} according to the relation

$$\frac{C_{p_i}}{R} = A + BT + CT^2 + DT^3 + ET^4 \quad (1)$$

These data were assimilated into mixture properties assuming ideal gas behavior for both thermal conductivity and specific heats.

$$k_{mix} = \sum_{i=1}^n y_i k_i \quad (2)$$

$$C_{p_{mix}} = \sum_{i=1}^n y_i C_{p_i} \quad (3)$$

For the mixture viscosity, this simple summation is inadequate and a method for the determination of mixture viscosities found in Walker² was utilized. Because of the property changes from air to an arbitrary chemical mixture, it was necessary to account for changes in the laminar recovery factor, turbulent recovery factor, laminar Reynolds analogy factor, and the turbulent Reynolds analogy factor.

The viscosity power law assumption was utilized in this investigation to determine the exponent, w , for use in the boundary layer calculations. This assumption is valid when $\ln \mu$ is linear with $\ln T$ as shown in Figure 1.



Figure 1. Viscosity as a function of temperature.

This linearity assumption was made in the program and the method of least squares was utilized to determine the slope w .

$$\frac{\mu}{\mu_0} = \left(\frac{T}{T_0} \right)^w$$

$$\ln \mu = \ln \mu_0 + w \ln \left(\frac{T}{T_0} \right) \quad (4)$$

$$e^{\ln \mu} = e^{w \ln \left(\frac{T}{T_0} \right) + c}$$

$$\mu = e^c \left(\frac{T}{T_0} \right)^w \quad (5)$$

Equation (5) was curve fit using a linear least squares routine. The coefficients c and w were evaluated utilizing (6) and (7).

$$w = \frac{\sigma_x \sigma_y - n \sigma_{xy}}{\sigma_x^2 - n \sigma_{xx}} \quad (6)$$

$$c = \frac{\sigma_y - b \sigma_x}{n} \quad (7)$$

The derivation of (6) and (7) is shown in Appendix A.

III. THE CODE

Subroutine NOAIR is the principal addition to COMPBL. If the program is run for a gas mixture other than air, Subroutine NOAIR is utilized.

Inputs into NOAIR include the Mach number and pressure, the elements comprising the mixture (along with the mole fraction of each), and the mixture temperature.

From these, the mixture viscosity is calculated at the input temperature by using the cubic spline interpolation routine mentioned before. Using this viscosity, the viscosity power law exponent is derived by using the least squares fit routine. Also, the specific heat ratio is found using the equation:

$$\gamma = \frac{C_{p_{mix}}}{C_{p_{mix}} - R} \quad (8)$$

The Prandtl number is also returned by the equation:

$$Pr = \left(\frac{\mu}{k} \right) \left(\frac{C_p}{R} \right) \left(\frac{1}{MW_{mix}} \right) \{1.98716\} \quad (9)$$

The Prandtl number is then used to change the laminar and turbulent recovery factors, as well as the laminar and turbulent Reynolds analogy factors:

$$\begin{aligned} RL &= Pr^{1/2} & SL &= Pr^{2/3} \\ RT &= Pr^{1/3} & ST &= Pr^{2/3} \end{aligned} \quad (10)$$

The density and velocity of flow also are calculated as follows:

$$\rho = \frac{p MW_{mix}}{T} \left[\frac{1}{8.3143} \right] \quad (11)$$

$$u = M \sqrt{\frac{\gamma R}{MW_{mix}} T} \quad (12)$$

These are used to calculate the Reynolds number.

$$Re = \frac{\rho u}{\mu} \quad (13)$$

A. Data Tapes

This program is designed to run on the CYBER 74 as well as run interactively on the INTERDATA 8/32. It is written in Standard Fortran IV.

Both versions contain three (3) DATA FILES within Subroutine NOAIR:

C1: Contains individual species viscosities for temperature range 200-3700°K.

COEF: Contains constant pressure specific heat coefficients taken from Program SPF DATABANK. (Used to calculate C_{p1}/R)

XKAY: Contains individual species thermal conductivity for temperature range 200-3700°K.

B. Arrangement of Data

To make Subroutine NOAIR function as simply as possible, it was necessary to arrange the data in a logical order. From the listing of elements, it is evident that the elements are in semi-alphabetical order, and are numbered as such.

These numbers are important, because the arrangement of the data (WTMOLE, C1, COEF, XKAY) also follow this order. In other words, for element N₂, the corresponding number is 31. Now, the molecular weight for N₂ is the 31st element in the array WTMOLE. The other three data files are also arranged in this way; however, in these latter data files, there are four lines of data per element for C1 and XKAY, and two lines of data per element in COEF, e.g., take N₂, number 31. The viscosities for temperature range 200-3700°K would be lines 121-124 in arrays C1 and XKAY and lines 61-62 in COEF (See Table I).

C. Adding New Elements

Taking the previous section into account, it is necessary to maintain this order. To add new elements, it should be easier to add the new element in position 47, and the data for WTMOLE, C1, COEF, XKAY should be attached to the end of each file.

Adding the new element will be a little different on the 8/32 and the CYBER 74. On the 8/32, the element will be added at the end of the listing:

43-0 44-02 45-03 46-0H 47-NEW

On the CYBER 74, the new element will be added on the end of the DATA Statement for ILEM:

DATA (ILEM(I), I = 1,50) 2HAR, 3HBCL, 4HBCL2, 4HBCL3,

.

.

.

\$1H0, 2H02, 2H03, 2H0H, 2HNE/

and the number 47 will be added to KLEM:

DATA (KLEM(K), K=1,50)/1,2,3,4,5,6,7,8,9,

.

.

.

\$44,45,46,47,3*0/

IV. DATA INPUT - CYBER BATCH VERSION

CARD 1: This card tells whether the boundary layer program is to run on properties of air or of another gas mixture

In Column 5, type

1 - for air

2 - for another mixture

CARD 2: (Only if '2' is typed on CARD 1)

Right Justify:

Columns 1-10: Mach or M* number

Columns 11-20: Pressure (in kilopascals)

(NOTE: Make sure pressure is entered in kilopascals).

CARD 3: (Only if '2' is typed on CARD 1)

Number of elements in the mixture

Right justify in columns 1-5.

CARD 4: (Only if '2' is typed on CARD 1)

These next cards contain information about the mixture.

Left justify in columns 1-6

Type in the element name

Right justify in columns 10-20

Type in the mole fraction of that element

(NOTE: Every element - mole fraction association must be on a separate card. There should be as many of these cards so to equal the number typed on Card 3. Also, mole fractions must add up to equal 1.0.)

CARD 5: (Only if '2' is typed on CARD 1)

Right justify in columns 1-10

Temperature of the mixture

(NOTE: Temperature must be entered as degrees Kelvin and the acceptable range is 200-3700°K.)

CARD 6: Right justify in Columns 1-80

Place the title of the boundary layer run. It is advised that this title be centered.

CARD 7: This card contains information necessary for boundary layer computations:

All are left justified

Columns 1-10: Enter the flow type (Laminar or Turbulent)

Columns 11-20: Enter geometry type (Plane 2-D or Axisym)

Columns 21-30: Enter velocity input data type (Mach or Mstar)

Columns 31-40: Enter wall temperature data (Theta or Twtinf)

CARD 8: This card is used to override the default values in Namelist BL.

Place a \$ in column 2 and the name of the namelist, type the name of the variable along with its new value, separate all variables by commas, end with \$.

Example:

1	2
\$ BL HSTART = 1.6, MINF = 0.308, G = 1.4\$	

CARD 9: The rest of the cards are data points necessary for boundary layer computations, as described in Dutton and Addy⁽¹⁾.

V. DATA INPUT - INTERDATA 8/32

In contrast to the CYBER Batch Version the INTERDATA 8/32 Version is interactive. The user utilizes a prompting system to input the data. The list of prompts and a description of each input follows:

1. Is this being run on a Tektronix Terminal?

Enter . Y . OR . N .

This question has to do with the terminal the program is run on. If "Y" is typed in, the screen will automatically clear itself when it is full.

2. Is this run to be based on the qualities of air? Enter Y or N.

If "Y" is entered, then Subroutine NOAIR is by-passed and the program utilizes the properties of air.

(NOTE: Questions 3-7 will appear ONLY if "N" is entered for question 2.)

3. Please enter Mach or Mstar Number.

Enter the Mach or M^{*} number. Be sure to include decimal point

Ex: > 0.9667

4. Please enter pressure in kilopascals

Enter the pressure in kilopascals. Be sure to include decimal point.

Ex: > 20. or 20.0

5. Now enter the number of elements in the gas mixture. The number can be between one and 99. If the number entered is one digit, include leading zero.

Ex: > 03 ; > 10

6. Here is a list of elements:

1-AR	2-BCL	3-BCL2	4-BCL3	5-BF	6-BF2
7-BF3	8-B0	9-B2O3	10-C	11-CH	12-C2H2
13-CH4	14-C2H4	15-CO	16-CO2	17-CL	18-CL2
19-CLF	20-CLF3	21-F	22-F2	23-H	24-H2
25-H2O	26-H2O2	27-HCL	28-HF	29-HE	30-N
31-N2	32-NF3	33-NH	34-NH3	35-NO	36-NO2
37-NOCL	38-N2O	39-NA	40-NACL	42-NAO	42-NAOH
43-O	44-O2	45-O3	46-OH		

Enter the corresponding number(s) of the elements to be used along with the mole fraction of each (i.e., 35% of O₃, enter 45,0.35)

These are all the elements contained in Subroutine NOAIR. Enter the element number, not the element name, along with the mole fraction of that element. Each prompt should contain the element number, followed by a comma and the elemental mole fraction. There will be as many prompts as the number entered for question 5.

Ex: for 35% of O₃: > 45, 0.35

(Mole fractions must add up to equal 1.0.)

7. Now enter the temperature of the mixture.

Enter the temperature of the mixture in degrees Kelvin. Be sure to include decimal point.

Ex: > 300.00

(Temperature must be within the range of 200-3700°Kelvin.)

The following cues appear regardless of the answer to question 2:

8. Enter type of flow:

Enter....LAMI....for Laminar

Enter....TURB....for Turbulent

Variable that describes the initial flow regime of boundary layer. Type in LAMI for laminar flow or TURB for turbulent flow.

9. Enter type of geometry:

Enter....2-D....for Plane 2-D

Enter....AXIS....for Axisymmetric

Variable that describes the geometry. Enter 2-D for plane 2-D or AXIS for axisymmetric.

10. Enter velocity data input type:

Enter....MACH....for Mach

Enter....MSTA....for Mstar (M^*)

Variable that describes whether velocity input data is in terms of Mach number or M^* ($=u/c^*$). Enter MACH for Mach number or MSTa for M^* .

11. Enter wall temperature input data:

Enter....THET....for Theta

Enter....TWTI....for Twinf

Variable that describes whether wall temperature input data is in terms of $\theta = [(T_e - T_w)/(T_e - T_A)]$ or T_w/T_∞ . Enter THET for theta (θ) or TWTI for T_w/T_∞ . (There are two prompts for the next question. Only one will appear and it depends on the answer to question 2).

12. The values for Mach or Mstar number, Reynolds number, Gamma, W, RL, RT, SL, ST, have been calculated. Here are the rest of the input variables:

ZSTART = 0.0000

HSTART = 1.572

BSTART = 0.0000

XTRAN = 0.0000

FST = 0.0000

EPS = 0.1000E-03

ERROR = F

NOTRAN = F

HCCORR = F

Do you wish to change any of the above?

Enter....Y....or....N....

This version appears if the answer to question 2 is "N".

Here are the input variables with their present (default) values:

ZSTART =	0.0000	
HSTART =	1.572	
BSTART =	0.0000	
MI =	0.0000	(MINF)
REINFL =	0.0000	
XTRAN =	0.0000	
FST =	0.0000	(FSTINT)
X =	1.405	(G)
W =	0.7000	
RL =	0.8500	
RTR =	0.8800	(RT)
SL =	0.8000	
STS =	0.8200	(ST)
EPS =	0.1000E-03	
ERROR =		F
NOTRAN =		F
HTCORR =		F

Do you wish to change any of the above?

Enter....Y....or....N....

This version appears if the answer to question 2 is "Y".

In either case, the question is designed to enable the user to override any of the default values for these variables. (See Figure 2 for explanation of the variables.) If new values are to be entered, type "Y"; if not, type "N".

Question 13 will appear only if answer to 12 is "Y".

(Two variables must be changed from 0.0 to another number; i.e., they must be given a value. These are MI (MINF) and REINFL, and need be changed only if question 12B appears.)

13. Enter names and new values (Name = New Value)

Enter them one at a time, pushing return after each or enter . % . to signal more variables to be changed.

>

> %

Enter the variable name followed by an equals sign and the new value. To terminate changes to these variables, type in "%".

Ex: > HSTART = 1.6

> MI = 1.0

> %

VI. SAMPLE INPUT

Sample Card Deck

Air Case

1					Whether run on air or not	
	GSRS BOUNDARY LAYER				1 - Air	
TURBULENT	AXISYM	MACH	THETA		Title of run	
\$BL HSTART=1.6,MINF=0.9667,REINFL=0.1081E6, G=1.397\$					Flow, geometry, velocity input data, wall temperature data Namelist BL	
0.0	1.888	1.0	1.888		Local data cards	
1.027	2.256	1.707	2.256			
2.197	2.792	2.11	2.792			
3.09	3.145	2.306	3.145			
4.3	3.5465	2.488	3.5465		XI, YI, MDI, RI	
5.222	3.802	2.589	3.802			
6.157	4.012	2.666	4.012			
6.63	4.1	2.696	4.1			
1	5	11	21	31	41	51

ZSTART--STARTING VALUE OF Z, [L] (DEFAULT=0.0)
 HSTART--STARTING VALUE OF H; SEE WALZ PP 267-268 AND FIGS I.1
 AND 6.5 AND ACCOMPANYING REPORT, TABLES I AND II
 AND FIG. 2 (DEFAULT=1.572)
 BSTART--BSTART*PI IS THE INCLUDED ANGLE AT THE LEADING EDGE
 FOR BOTH PLANE 2-D AND AXISYMMETRIC EXTERNAL FLOWS
 (DEFAULT=0.0)
 MINF----MACH NUMBER (OR MSTAR) OF APPROACH FLOW
 REINFL--REYNOLDS NUMBER DIVIDED BY CHARACTERISTIC LENGTH OF
 APPROACH FLOW, I.E. $\rho_{\infty} U_{\infty} / \mu_{\infty}$, [L]**(-1)
 XTRAN---X LOCATION FOR SPECIFIED TRANSITION, [L]
 (DEFAULT=0.0)
 PSTINT--FREESTREAM TURBULENCE INTENSITY--USED IN TRANSITION
 SUBROUTINE, IN PERCENT (DEFAULT=0.0)
 G-----RATIO OF SPECIFIC HEATS (DEFAULT=1.405)
 W-----EXPONENT ON VISCOSITY POWER LAW (DEFAULT=0.7)
 RL-----LAMINAR RECOVERY FACTOR (DEFAULT=0.85)
 RT-----TURBULENT RECOVERY FACTOR (DEFAULT=0.88)
 BL-----LAMINAR REYNOLDS ANALOG FACTOR (DEFAULT=0.80)
 ST-----TURBULENT REYNOLDS ANALOG FACTOR (DEFAULT=0.82)
 EPS-----CONVERGENCE CRITERION VARIABLE (DEFAULT=1.0E-4)
 NOTRAN--LOGICAL VARIABLE WHICH IF .TRUE. SUPPRESSES
 CALLING OF THE TRANSITION SUBROUTINE FOR LAMINAR
 BOUNDARY LAYERS (DEFAULT=.FALSE.)
 HTCORR--LOGICAL VARIABLE WHICH IF .TRUE. CAUSES THE THERMAL
 ENERGY INTEGRAL EQUATION TO BE SOLVED FOR THE HEAT
 FLUX CORRECTION PARAMETER, CHT (DEFAULT=.FALSE.)
 ERROR---LOGICAL VARIABLE WHICH IF .TRUE. CAUSES INTERMEDIATE
 H VALUES AND VARIABLES ASSOCIATED WITH THE TURBULENT
 DISSIPATION INTEGRAL AND HEAT TRANSFER CORRECTION
 PARAMETER TO BE PRINTED FOR DEBUGGING PURPOSES
 (DEFAULT=.FALSE.)

Figure 2. Explanation of variables for question 12.

Sample Card Deck

N₂/O₂ Case

2					Whether run on air or not
0.967	20.0				2 - Not air
2					Mach Number - Pressure
N2	0.79				Number of elements in mixture
O2	0.21				Element/Mole Fraction
300.00					Temperature of mixture
GSRS BOUNDARY LAYER					Title of Run
TURBULENT	AXISYM	MACH	THETA		Flow, geometry, velocity input data, wall
\$BL HSTART =1.6\$					temperature data
0.0	1.888	1.0	1.888		Namelist BL
.	.	.	.		Local data cards
.	.	.	.		XI, YI, MDI, RI, THETI
6.63	4.1	2.696	4.1		NOTE:
					(Same as Air Case above)
1	5	11	21	31	41
					51

XI---Axial Location, [L]

YI---Normal Location, [L]

MDI---Freestream Mach Number (or MSTAR)

RI---Cross-Sectional Radius of Axisymmetric Bodies, or
Location Normal to Centerline for 2-D Bodies [L]

THETI---Wall Temperature Ratio $(T_{adwall}-T_{wall})/(T_{adwall}-T_{stream})$ or T_{wall}/T_{INF} -

VII. SAMPLE OUTPUT

A. Sample Case Using Air

B. Sample Case Using N₂/O₂

COMPRESSIBLE BOUNDARY LAYER RESULTS--COMPUTATIONAL METHOD II OF WALZ

GEPS BOUNDARY LAYER(VOUGHT/ARC PROPELLANT)(L=MIN.)

INPUT PARAMETERS:

FLOW = TURB
 TYPE = THET
 HSTART = 0.0000
 XTHAN = 0.0000
 W = 0.7000
 SL = 0.8000
 MOTRAN = F

 GEOM = AXIS
 ZSTART = 0.0000
 MINF = 0.9666
 FSTINT = 0.0000
 RL = 0.8500
 ST = 0.8200
 WTCORR = F

 MTYPE = MACH
 HSTART = 1.600
 REINFL = 0.1081E+06
 G = 1.397
 RT = 0.8800
 EPS = 0.1000E-03
 ERROR = F

RESULTS:

AXIAL LOCATION (L)	Z = D2*(R02**N) (L)	H = (D3/D2)U (L)	SHAPE FACTOR (D1/D2)	DISPLACEMENT THICKNESS (L)	MOMENTUM THICKNESS (L)	99.9% B.L. THICKNESS (L)	NOM. THICK. REYNOLDS NUMBER	LOCAL SKIN FRICTION COEFFICIENT	DIMENSIONLESS LOCAL WALL HEAT FLUX
0.000000	0.000000	1.60000	----	0.000000	0.000000	0.000000	0.000000	----	----
1.02700	0.165435	1.60000	3.90076	0.582092E-02	0.149225E-02	0.199354E-01	110.862	0.410358E-02	0.000000
LAMINAR-TURBULENT TRANSITION									
2.19700	0.139742E-01	1.70179	3.35856	0.115726E-01	0.344571E-02	0.327260E-01	185.709	0.433045E-02	0.000000
3.09000	0.201116E-01	1.70265	3.71985	0.178470E-01	0.479777E-02	0.479850E-01	217.998	0.396326E-02	0.000000
4.30000	0.285533E-01	1.70423	4.08005	0.265147E-01	0.649861E-02	0.683960E-01	250.403	0.366956E-02	0.000000
5.22200	0.347700E-01	1.70400	4.29660	0.332639E-01	0.774192E-02	0.836389E-01	271.748	0.349163E-02	0.000000
6.15700	0.411700E-01	1.70396	4.46661	0.401121E-01	0.898042E-02	0.990082E-01	293.412	0.335097E-02	0.000000
6.63000	0.445032E-01	1.70341	4.53682	0.435799E-01	0.960583E-02	0.108629	305.167	0.328072E-02	0.000000

Figure A. Sample output of COMPEL-II based on properties of air. (Subroutine NOAIR not used.)

COMPRESSIBLE BOUNDARY LAYER RESULTS--COMPUTATIONAL METHOD II OF WALL

GSR5 BOUNDARY LAYER(VOUGHT/ARC PROPELLANT)(USIN.)

INPUT PARAMETERS:

FLOW = TURB
 TYPE = THET
 HSTART = 0.0000
 XTRAN = 0.0000
 h = 0.6923
 SL = 0.7835
 NOTRAN = F

GEOM = AXIS
 ZSTART = 0.0000
 KINF = 0.9666
 PSTINT = 0.0000
 RL = 0.8312
 ST = 0.7835
 WTCORR = F

WTYPE = MACH
 HSTART = 1.600
 REINFL = 0.1074E+06
 G = 1.397
 RT = 0.8851
 EPS = 0.1000E-03
 ERROR = F

RESULTS:

AXIAL LOCATION (L)	Z = D24(R02*H) (L)	h = (D3/D2)U	SHAPE FACTOR (01/02)	DISPLACEMENT THICKNESS (L)	MOMENTUM THICKNESS (L)	99.9(B.L. THICKNESS (L)	NON. THICK. REYNOLDS NUMBER	LOCAL SKIN FRICTION COEFFICIENT	DIMENSIONLESS LOCAL WALL HEAT FLUX
0.00000	0.000000	1.60000	----	0.000000	0.000000	0.000000	0.000000	----	----
1.02700	0.166276	1.60000	3.86753	0.578646E-02	0.149616E-02	0.198864E-01	111.135	0.411433E-02	0.000000
LAMINAR-TURBULENT TRANSITION									
2.19700	0.139463E-01	1.70170	3.37021	0.116116E-01	0.344536E-02	0.327685E-01	184.399	0.432992E-02	0.000000
3.09000	0.202567E-01	1.70253	3.73383	0.179030E-01	0.478481E-02	0.480297E-01	216.305	0.396219E-02	0.000000
4.30000	0.284614E-01	1.70410	4.09631	0.265945E-01	0.649230E-02	0.684461E-01	248.326	0.366810E-02	0.000000
5.22200	0.346511E-01	1.70385	4.31424	0.333629E-01	0.773319E-02	0.836942E-01	269.427	0.348986E-02	0.000000
6.15700	0.410231E-01	1.70380	4.48534	0.402306E-01	0.896937E-02	0.990696E-01	290.857	0.334901E-02	0.000000
6.63000	0.443422E-01	1.70325	4.55599	0.437088E-01	0.959369E-02	0.106694	302.493	0.327866E-02	0.000000

Figure B. Sample output of COMBL-II based on properties of air.
 (Subroutine NOAIR used for air composition of 79% N2 and
 21% O2)

TABLE I. SAMPLE FROM DATA TABLES ILLUSTRATING N₂

0.24502680E+01	0.10661460E-03	-0.74653370E-07	0.18796520E-10	-0.10259840E-14	N
0.25030720E+01	-0.21800180E-04	0.54205290E-07	-0.56475600E-10	0.20999040E-13	
0.28963190E+01	0.15154870E-02	-0.57235280E-06	0.99807400E-10	-0.65223570E-14	N ₂
0.36748260E+01	-0.12081500E-02	0.23240100E-05	-0.63217570E-09	-0.22577250E-12	
0.79819180E+01	0.22349900E-02	-0.96301030E-06	0.18357810E-09	-0.12901440E-13	NF ₃
0.12676910E+01	0.24289230E-01	-0.26835970E-04	0.11994190E-07	-0.12905660E-11	

ARRAY COEF. ELEMENTAL CONSTANT PRESSURE SPECIFIC HEAT COEFFICIENTS

123.1	166.6	203.7	237.0	267.6	296.0	322.6	347.9	372.3	N
396.4	419.9	442.4	464.3	485.6	506.4	526.7	546.6	566.1	
585.2	603.9	622.4	640.5	658.3	675.9	693.2	710.3	727.2	
743.8	760.3	776.5	792.6	808.5	824.2	839.7	855.1	870.4	
131.3	177.7	217.2	252.7	285.4	315.6	344.0	371.0	397.1	N ₂
422.7	447.8	471.8	495.2	517.9	540.1	561.7	582.9	603.7	
624.0	644.0	663.7	683.0	702.1	720.8	739.3	757.5	775.5	
793.3	810.8	828.1	845.3	862.2	879.0	895.5	912.0	928.2	
124.0	181.7	232.4	277.7	319.1	357.3	393.1	426.7	458.7	NF ₃
489.5	519.1	547.8	575.5	602.3	628.4	653.7	678.3	702.4	
725.9	749.0	771.6	794.0	816.1	838.0	859.8	881.5	903.3	
924.3	945.0	965.5	985.7	1005.7	1025.5	1045.0	1064.3	1083.5	

ARRAY C1. ELEMENTAL VISCOSITIES

65.5	88.6	108.4	126.1	142.4	157.5	171.6	185.1	198.1	N
210.9	223.4	235.4	247.0	258.4	269.4	280.2	290.8	301.2	
311.4	321.4	331.3	341.0	350.6	360.2	369.7	397.1	388.6	
398.0	407.5	417.0	426.6	436.3	446.1	456.0	466.1	476.3	
47.2	63.9	78.5	92.2	105.9	119.4	132.7	145.9	158.9	N ₂
171.7	184.3	196.4	208.2	219.7	230.8	241.6	252.2	262.5	
272.6	282.4	292.1	301.6	310.9	320.0	329.0	337.9	346.6	
355.2	363.6	372.0	380.3	388.4	396.5	404.5	412.3	420.2	
24.7	45.0	66.2	86.3	104.8	121.7	137.3	151.7	165.2	NF ₃
178.0	190.2	201.9	231.2	224.0	234.4	244.5	254.3	263.8	
273.1	282.2	291.0	299.8	308.4	317.0	325.5	333.9	342.4	
350.5	358.5	366.5	374.3	382.0	389.6	397.2	404.6	412.0	

ARRAY XKAY. ELEMENTAL THERMAL CONDUCTIVITIES

VIII. RESULTS AND CONCLUSIONS

A boundary layer program has been modified to account for arbitrary chemical composition flow streams. This program can be run in two different modes:

1. Interactively, on the INTERD, TA 8/32 for design calculations.
2. Batch, on the CYBER for multiple runs and in conjunction with other codes.

A sample case is given in the Appendix which is the same case as given in the original COMPBL documentation. The difference is that this analysis specifies the chemical composition of air in order to indicate the new capabilities added to the code.

These improvements add the capability of analyzing internal flows for aeropropulsion applications such as nozzles and diffusers.

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3. Svehla, R. A., "Estimated Viscosities and Thermal Conductivities of Gases at High Temperatures," NASA Technical Report R-132, Lewis Research Center, Cleveland, Ohio, 1962.
4. Walker, B. J., "Calculation of the Laminar Viscosity of a Gaseous Mixture for Gas Dynamic Mixing Comparisons for a Reacting Shear Layer," MICOM Technical Report RD-80-2, Redstone Arsenal, Alabama, October 1979.
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APPENDIX A
LINEAR LEAST SQUARES FIT

For a given linear function $y(x)$ given by (A1)

$$y = a + bx \quad (A1)$$

The residuals are given by v_1

$$\begin{aligned} v_1 &= a + bx_1 - y_1 \\ v_2 &= a + bx_2 - y_2 \end{aligned} \quad (A2)$$

$$v_n = a + bx_n - y_n$$

In order to determine the best fit, the sum of the squares of the residuals is a minimum

$$\sum v^2 = v_1^2 + v_2^2 + \dots + v_n^2 \quad (A3)$$

$$\begin{aligned} \sum (a+bx-y)^2 &= (a+bx_1-y_1)^2 + (a+bx_2-y_2)^2 \dots + (a+bx_n-y_n)^2 \\ &= f(a,b) \end{aligned} \quad (A4)$$

For $f(a,b)$ to a minimum

$$\frac{\partial f}{\partial a} = 2(a+bx_1-y_1)(1) + 2(a+bx_2-y_2)(1) + \dots + 2(a+bx_n-y_n)(1) = 0 \quad (A5)$$

$$\frac{\partial f}{\partial b} = 2(a+bx_1-y_1)x_1 + 2(a+bx_2-y_2)x_2 + \dots + 2(a+bx_n-y_n)x_n = 0 \quad (A6)$$

Dividing (A5) and (A6) by 2

$$\frac{\partial f}{\partial a} = (a+bx_1-y_1) + (a+bx_2-y_2) + \dots + (a+bx_n-y_n) = 0 \quad (A7)$$

$$\frac{\partial f}{\partial b} = (a+bx_1-y_1)x_1 + (a+bx_2-y_2)x_2 + \dots + (a+bx_n-y_n)x_n = 0 \quad (A8)$$

Rewriting (A7) and (A8)

$$na + \sum_{i=1}^n x_i b = \sum_{i=1}^n y_i \quad (A9)$$

$$\sum_{i=1}^n x_i a + b \sum_{i=1}^n x_i^2 = \sum_{i=1}^n x_i y_i \quad (A10)$$

Solving for a and b from (A9) and (A10)

$$a = \frac{\sum_{i=1}^n x_i y_i - b \sum_{i=1}^n x_i^2}{\sum_{i=1}^n x_i} \quad (A11)$$

$$b = \frac{\sum_{i=1}^n y_i - na}{\sum_{i=1}^n x_i} \quad (A12)$$

Substituting for a in (A9)

$$\frac{n\sigma_{xy} - nb\sigma_{xx}}{\sigma_x} + b\sigma_x = \sigma_y \quad (A13)$$

$$n\sigma_{xy} - nb\sigma_{xx} + b\sigma_x^2 = \sigma_x\sigma_y \quad (A14)$$

$$b(\sigma_x^2 - n\sigma_{xx}) = \sigma_x\sigma_y - n\sigma_{xy}$$

Hence

$$b = \frac{\sigma_x\sigma_y - n\sigma_{xy}}{\sigma_x^2 - n\sigma_{xx}} \quad (A15)$$

from (A9)

$$a = \frac{\sigma_y - b\sigma_x}{n} \quad (A16)$$

where:

$$\sigma_x = \sum_{i=1}^n x_i \quad \sigma_y = \sum_{i=1}^n y_i \quad (A17)$$

$$\sigma_{xx} = \sum_{i=1}^n x_i^2 \quad \sigma_{xy} = \sum_{i=1}^n x_i y_i$$

Equations (A15) - (A17) are utilized to determine the linear least squares curve fit.

APPENDIX B

SAMPLE CASE - AIR VERSUS N_2/O_2

In order to test the reliability of the boundary layer computations on a given gas mixture, it was necessary to run a sample case. In Case I, the boundary layer program was run in its original form (that is, based on air) and Subroutine NOAIR was not used. In Case II, Subroutine NOAIR was used, based on a mixture of 79% N₂ and 21% O₂, the accepted composition of air.

It was, therefore, necessary to arrange all input data for both cases to be as near alike as possible. Subroutine NOAIR had been found to work on the N₂/O₂ mixture at a temperature of 300°. (That is, the mixture viscosity, the ratio of specific heats, viscosity power law exponent, and the Prandtl number all were correct.) Therefore, it was easier to change the inputs of Program COMPBL (without Subroutine NOAIR).

CALCULATION OF SAMPLE DATA:

Three variables in Program COMPBL had to be calculated so that the program could be tested. These were MINF, REINFL, and G.

To get MINF, the equation $MINF = u/a$ was used. An arbitrary u was chosen to be 1100 ft/sec (335.28 m/s). The value for a was calculated following

$$a = \sqrt{\frac{\gamma RT}{MW}}$$

The temperature, T , was input as 300°K.

Gamma (G) was previously calculated to be 1.397, therefore,

$$a = \sqrt{\frac{(1.397)(8314.3 \text{ J/K MOLE} - ^\circ\text{K})(300^\circ\text{K})}{28.96 \text{ kg}}}$$

$$\text{So: } a = 346.8745$$

$$\text{and } MINF = 335.28/346.8745$$

$$MINF = .96657$$

In order to calculate REINFL, the equation

$$REINFL = \frac{\rho u}{\mu} \quad \text{or} \quad REINFL = \left(\frac{PMW}{RT} \right) \frac{u}{\mu}$$

was utilized, using input temperature of 300°K and input pressure of 20 kilopascals. The viscosity, μ , was found for air using the following equation taken from Reference 5.

$$\mu = 2.27 \frac{T^{3/2}}{T+198.6} \times 10^{-3} \frac{\text{lb}_m \text{ SEC}}{\text{ft}^2}$$

For $T = 300^\circ\text{K}$ and SI units

$$\mu = 8.295 \times 10^{-7} \text{ kg s/m}^2$$

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